Database Presenting Basic Information about EU WFD Priority Substances

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Database Presenting Basic Information about EU WFD Priority Substances

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Source Control Options for Reducing Emissions of Priority Pollutants (ScorePP)

Sixth Framework Programme, Sub-Priority 1.1.6.3, Global Change and Ecosystems

Project no. 037036, www.scorepp.eu, Duration: 1 October 2006 – 30 September 2009

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Abstract (max. 200 words)

The aim of task 3.1 was to construct a database that is able to support the consortium in the other tasks and work packages with basic information regarding the priority pollutants.

Basic information regarding inherent properties, environmental fate, risk classifications, observations in the environment and present legislation have been compiled for 67 chemicals and chemical groups. These 67 chemicals and chemical groups are included in the Water Framework Directive.

The database is constructed in MS Access, and within the database there are several forms to handle chemicals, properties, data sources and data entries. In order to retrieve data from the database, an add-on program is used to generate a report in MS Excel based on the data in the database. Data on all properties for one chemical or data on all chemicals for one property are examples of the kind of reports that may be generated from the database.

Acknowledgement

The presented results have been obtained within the framework of the project ScorePP - “Source Control Options for Reducing Emissions of Priority Pollutants”, contract no. 037036, a project coordinated by Institute of Environment & Resources, Technical University of Denmark within the Energy, Environment and Sustainable Development section of the European Community’s Sixth Framework Programme for Research, Technological Development and Demonstration.

Table of Contents

1. Introduction

The output from task 3.1 is a database with data on basic information of the chemicals listed on the Water Framework Directive (WFD) (EC, 2001). As a start there were only 33 priority pollutants on the WFD, but later on a list with environmental quality standards was proposed by EU, including some additional chemicals (EC, 2006). Further, the metals listed on the WFD not only include the metallic and ionic forms but also some of the organo-metallic derivatives. Therefore, a total of 67 chemicals are included in the present database. The basic information compiled comprises inherent properties, environmental fate, risk classifications, observations in the environment and present legislation. Data were compiled from various data sources as handbooks, Internet databases and original literature, cf. References.

MS Access was selected as the database software. A lot of effort has been put into constructing the database structure, the forms used to enter information into the database as well as producing an interface (an add-on program) enabling easy retrieval of the content of the database. In the database there are thus several forms in order to establish, enter and manage chemicals, properties, data sources, data entries and data retrieval, cf. Appendix A.

The results obtained in this task (selected chemicals, which parameters to compile information about and the functionality of the constructed database) are presented in a PowerPoint-presentation, cf Appendix B. The reason for choosing a PowerPoint-presentation rather than a traditional report as the communication media was that it gives an opportunity for making a more interactive presentation where the reader is able to go through the whole presentation from one end to the other *or* only read selected parts of interest. The latter part is established through the use of slides with short cuts to subsections of the presentation. In addition it was found easier to show the functionality of the database in a PowerPoint-presentation rather than a text file.

Also included in this deliverable is a compilation of the present legislation in EU and Sweden and a comprehensive overview of the phase distribution data, viz. presence data in both water and solid phases. Both legislation and presence data are compiled in spreadsheets and a report with detailed information about the presence data is found as a text file, cf. Appendix C.

2. Requirements When Using the Database

When using the database it is required to have MS Access and MS Excel installed on the computer's hard drive. Windows must also be upgraded with MS.Net FrameWork 2.0. Data are retrieved from the database by using an add-on programme; ReportGenerator. There is a direct link in the database to this ReportGenerator. The ReportGenerator must also be installed on the hard drive in the same folder as the database.

3. References

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ENVICAT Consulting, Avenue Montesquieu 36, B-1300 Wavre, Belgium.

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US National Library of Medicine (2006). Hazardous Substance Data Bank (HSDB). http://www.toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB (accessed 15 July 2007).

4. Appendices

Appendix A:

- PowerPoint-presentation with introduction to the database (Filename: **D3.1 - Short introduction to using the Database presenting basic information about EU WFD priority substances**).
- Database (filename: **D3.1 - Database presenting basic information about EU WFD priority substances - ed. 6.5.0**).
- Add-on programme (filename: **ReportGenerator**).
- Link to .NET FrameWork 2.0: http://www.microsoft.com/downloads/details.aspx?FamilyID=0856EACB-4362-4B0D-8EDD-AAB15C5E04F5&displaylang=en.

Appendix B:

- PowerPoint-presentation of the results obtained in this task (filename: **D3.1 - Database presenting basic information about EU WFD priority substances**).

Appendix C:

- Spreadsheets with legislation data (filename: **D3.1 - Legislation**).
- Spreadsheets with phase distribution data (filename*: **XXX - Phase distribution data**).
- Text file with report on detailed information about presence data (filename: **Phase distribution data report for Task 3.1**).

*: XXX represents the name of the various chemicals.

The above mentioned PowerPoint-presentations, database, software and documents including this report can all be downloaded from the ScorePP website at http://www.scorepp.eu/asp.net/.

5. Review and Assessment

After submitting the deliverable in September 2007 it was found that the layout of the database reports could be better, negative values representing text strings reported in the database were misleading and that a short guideline to using the database also was missed.

During the autumn 2007 the report layouts were therefore changed and negative values in the reports were replaced by the text strings they represented and a short guideline to using the database was established in a PowerPoint format.

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Source Control Options for Reducing Emissions of Priority Pollutants (ScorePP)

D3.1 Compilation of PP Inherent Properties

Structure of this deliverable

Objective | Intention | Participants

Overview

Structure of this deliverable

- This deliverable functions as a normal PowerPoint presentation. However, in order to make it more dynamic and interactive it is possible on every slide to jump directly to the last slide viewed and to the front page. In addition there are some slides which have an overview structure. Here it is possible to jump directly to the subject of interest.

Objective

- The objective of this task was to collect basic information regarding inherent properties, environmental fate and presence and legislation for the substances identified in the Water Framework Directive (WFD).

  The majority of this information has been established in an MS Access database for the purpose of easy sharing of information within the consortium.

Intention

- The intention for this task was to collect sufficient data for each property for each chemical. Thus, where possible, more than one value has been reported for each property, but in cases where many values were found this was limited to a selection of representative values.
- Various databases available on the Internet have been searched to obtain the information presented in this collection of data, however, with respect to the environmental presence data, original literature was also searched.
- Information about the quality of the data was also reported, including details about the experiment and the kind of reference cited (i.e. database or original literature).

Task participants

- The Danish Technical University (lead)
  - Eva Eriksson, Hans-Christian Holten Lützhøft (task leader) and Anna Ledin (work package leader)
- Middlesex University (contributor and review&assessment)
  - Erica Donner and Lian Scholes
- ENVICAT Consulting (contributor)
  - André Lecloux
- City of Stockholm (contributor)
  - Tonie Wickman
- Database collaborators
  - Stine Søndergaard, Mikkel Faarup and Khara Deanne Grieger

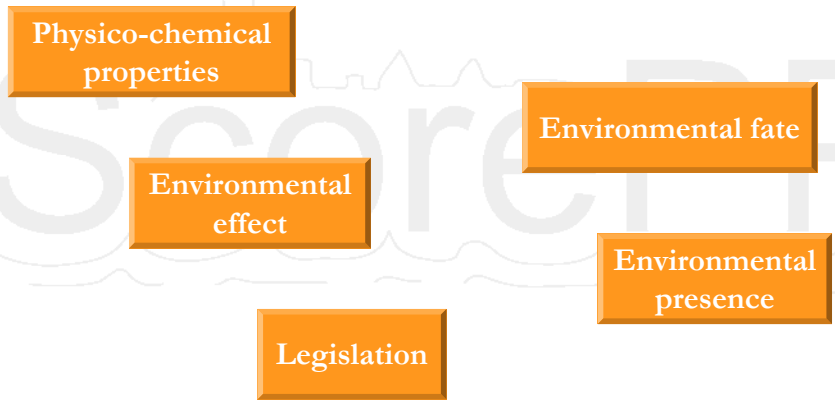
Overview

Information included in the database

Substances identified in the Water Framwork Directive

The database

Information included in the database



Physico-chemical properties

- Chemical Ids; CAS#, EINECS, Merck #
- Molecular formula
- Physical appearance
- Density (n), g/mL
- Molecular weight (M_w), g/mole
- Melting point (T_m), °C
- Boiling point (T_b), °C
- Solubility in water (S_w), mg/L
- Lipid solubility of neutral species (log K_{OW})
- Lipid solubility of ionized species (log D_{OW})
- Vapour pressure, mm Hg
- Acid dissociation constant (pK_a)
- Henry's law constant (KH), atm×m^3/mole
- Diffusion coefficient, m^2/d

Environmental fate

- Distribution between organic carbon and water (K_{OC}), L/kg
- Distribution between solids and water (K_D), L/kg
- Complexformation (K_C)
- Photodegradation ($t_{½}$), d
- Oxidation ($t_{½}$), d
- Hydrolysis ($t_{½}$), d
- Aerobic biodegradation ($t_{½}$), d
- Anaerobic biodegradation ($t_{½}$), d
- Yield of growth on chemical

Environmental effect

- Environmental Quality Standards (EQS) according to Proposal for a Directive of the European Parliament and of the Council on environmental quality standards in the field of water policy and amending Directive 2000/60/EC

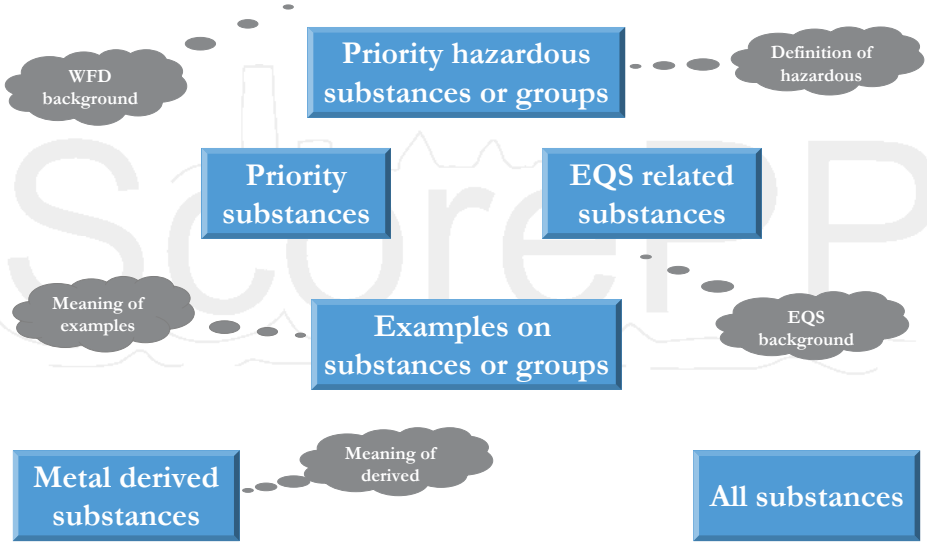
Environmental presence

- Surface water; rivers, lakes, harbours, streams, lagoons, wetlands, canals, reservoirs, estuaries etc.
- Porewater (soil or sediment)
- Suspended sediment
- Sediment
- Soil

Legislation/regulations

- EU legislation
- Case city country legislation
- Risk and safety phrases
- Classification
- Symbols
- Peak concentration limits
- Average concentration limits
- Restricted use
- Ban

Substances identified in the Water Framework Directive



Background of the substances on the Water Framework Directive

- In the mid 1990s a starting list of 268 substances was chosen for further consideration based on the work of previous forums (this initial list was selected more on the basis of politics than on scientific grounds).
- The substances were then ranked according to their measured concentrations or estimated concentrations (using production and use pattern, MacKay level 1 modelling and biodegradation) in water or sediment and predicted no-effect concentrations, bio-concentration factors and carcinogenic, mutagenic and reprotoxic data.

➢ This work resulted in the WFD with a list of 33 priority substances.

Background of the proposal on environmental quality standards

- **"Article 16 of the Water Framework Directive 2000/60/EC (WFD) sets out a strategy for dealing with chemical pollution in water. As a first step of this strategy, a list of priority substances was adopted (Decision 2455/2001/EC) identifying 33 substances of priority concern at Community level. This proposal aims to ensure a high level of protection against risks to or via the aquatic environment stemming from these 33 priority substances and certain other pollutants by setting environmental quality standards (EQS). The necessary emission controls have been adopted in various Community acts over the past years." (EQS).**

Definition of priority (hazardous) substances and meaning of examples

- **Priority substance: The work on identifying a range of substances resulted in the WFD where 33 substances or groups of substances were identified according to their exposure and effect data (see WFD background on the previous slide).**
- **Priority *hazardous* substance: To decide whether a particular priority substance should be classified as hazardous or not, the substance's persistence, bioaccumulation and toxicity data were evaluated according to certain criteria. 11 substances were identified on the WFD, but in relation to the EQS directive also anthracene and endosulfan have been proposed to be added to the list of priority hazardous substances.**
- **Examples: Both on the WFD and the following proposal to EQS some substance groups are mentioned including one or more specific substance(s) belonging to this group, e.g. trichlorobenzenes are mentioned on the WFD and 1,2,4-trichlorobenzene is given as an example.**

How the organometallic substances were derived

- The metals on the WFD list of substances are listed as e.g. “Lead and its compounds”
- In this task the participants have agreed to extend the list to include some of the many organometallic substances as well on the ionic species.
- The selected organometallic substances were chosen according to their relevance as they appeared in the US National Library of Medicine, Toxnet - Hazardous Substances Data Bank and through expert judgements made by the participants

The 33 priority substances

Alachlor

Anthracene
Atrazine
Benzene
Brominated diphenylethers
Cadmium and its compounds

C_{10-13}-chloroalkanes
Chlorfenvinphos
Chloroform
Chlorpyrifos

DEHP
1,2-dichloroethane
Dichloromethane

Diuron
Endosulfan

Fluoranthene
Hexachlorobenzene
Hexachlorobutadiene
Hexachlorocyclohexane

Isoproturon
Lead and its compounds

Mercury and its compounds

Naphthalene
Nickel and its compounds
Nonylphenols

Octylphenols

Pentachlorobenzene
Pentachlorophenol
Polyaromatic hydrocarbons

Simazine

Tributyltin compounds

Trichlorobenzenes

Trifluralin

The 8 substances related to the EQS

Aldrin

Carbontetrachloride

para-para'-DDT

Dieldrin

Endrin

Isodrin

Tetrachloroethylene

Trichloroethylene

Examples on substances or groups

Hexachlorocyclohexane
gamma-isomer, Lindane

para-para'-DDT
orto-para'-DDT
para-para'-DDE
para-para'-DDD

Endosulfan
Alpha-endosulfan

Nonylphenols
4-(para)nonylphenol

Octylphenols
Para-tert-octylphenol

Polyaromatic hydrocarbons
Benzo(a)pyrene
Benzo(b)fluoranthene
Benzo(g,h,i)perylene
Benzo(k)fluoranthene
Indeno(1,2,3-cd)pyrene

Tributyltin compounds
Tributyltin-cation

Trichlorobenzenes
1,2,4-trichlorobenzene

The 11 priority hazardous substances or groups

Hexachlorobenzene
Hexachlorobutadiene
Hexachlorocyclohexane

Pentachlorobenzene

Polyaromatic hydrocarbons

Brominated diphenylethers
Cadmium and its compounds

C_{10-13}-chloroalkanes

Tributyltin compounds

Mercury and its compounds

Nonylphenols

The metal derived substances

Lead and its compounds
Diethyldimethyllead
Ethyltrimethyllead
Methyltriethyllead
Tetraethyl lead
Tetramethyl lead

Tributyltin compounds

Mercury and its compounds
Diethylmercury
Dimethylmercury
Methylmercury
Phenylmercuric acetate

Bis(tributyltin) oxide
Tetra-N-Butyltin
Tributylchlorostannane
Tributyltin methacrylate

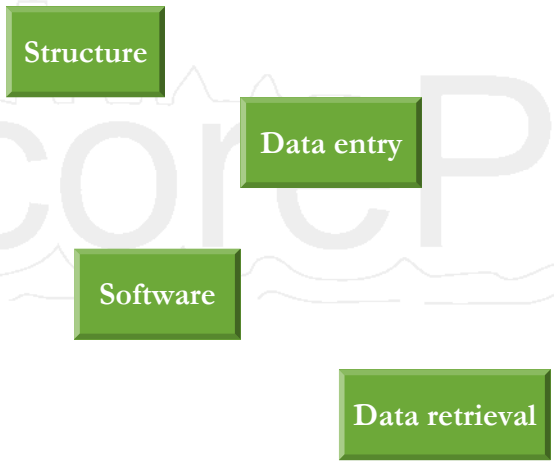
All 67 substances

Alachlor
Aldrin
Anthracene
Atrazine
Benzene
Brominated diphenylethers
Cadmium and its compounds
Carbontetrachloride
C_{10-13}-chloroalkanes
Chlorfenvinphos
Chloroform
Chlorpyrifos
para-para'-DDT
orto-para'-DDT
para-para'-DDE
para-para'-DDD
DEHP
1,2-dichloroethane
Dichloromethane
Dieldrin
Diuron
Endosulfan
Alpha-endosulfan

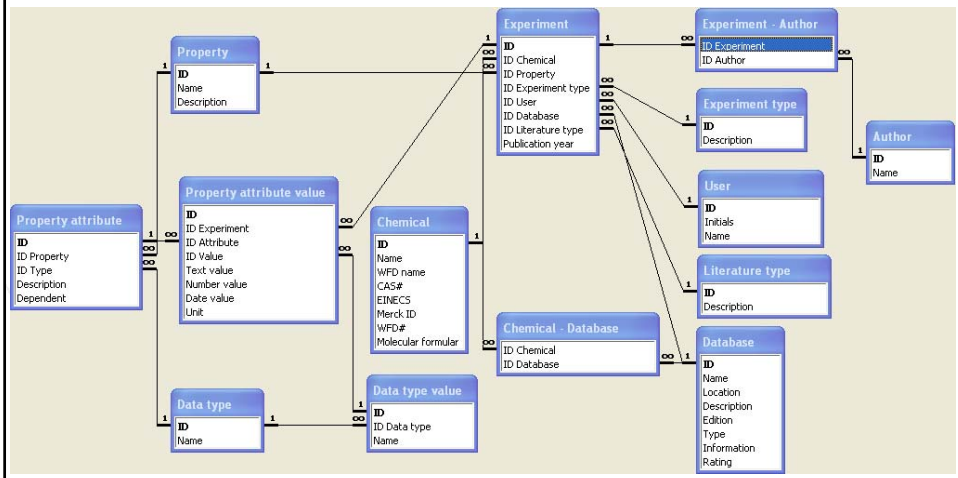
Endrin
Fluoranthene
Hexachlorobenzene
Hexachlorobutadiene
Hexachlorocyclohexane
gamma-isomer, Lindane
Isodrin
Isoproturon
Lead and its compounds
Diethyldimethyllead
Ethyltrimethyllead
Methyltriethyllead
Tetraethyl lead
Tetramethyl lead
Mercury and its compounds
Diethylmercury
Dimethylmercury
Methylmercury
Phenylmercuric acetate
Naphthalene
Nickel and its compounds
Nonylphenols
4-(para)nonylphenol

Octylphenols
Para-tert-octylphenol
Pentachlorobenzene
Pentachlorophenol
Polyaromatic hydrocarbons
Benzo(a)pyrene
Benzo(b)fluoranthene
Benzo(g,h,i)perylene
Benzo(k)fluoranthene
Indeno(1,2,3-cd)pyrene
Simazine
Tetrachloroethylene
Tributyltin compounds
Tributyltin-cation
Bis(tributyltin) oxide
Tetra-N-Butyltin
Tributylchlorostannane
Tributyltin methacrylate
Trichlorobenzenes
1,2,4-trichlorobenzene
Trichloroethylene
Trifluralin

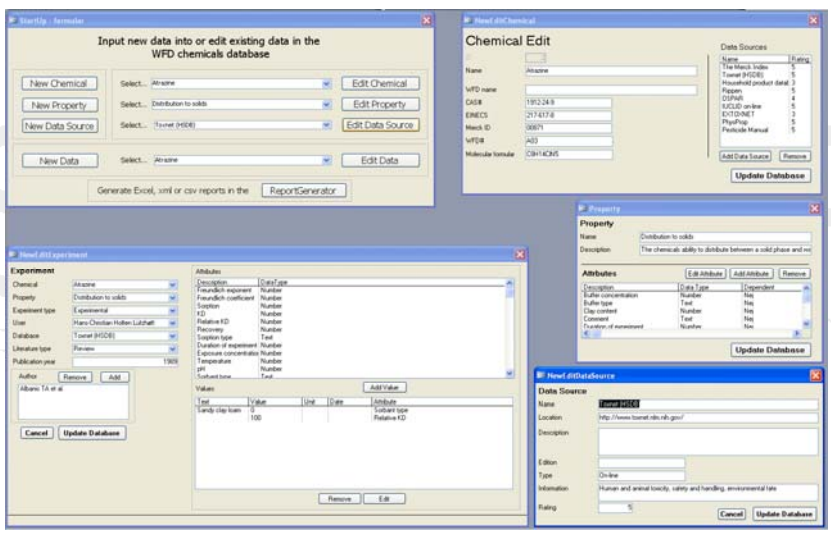
The database



Structure and relationships



Data entry



Click on a form to get more information!

Main entry form

- This form presents the various possibilities in the database
  - Selecting records for review or editing on
    - existing chemicals
    - properties
    - data sources
    - data
  - Creating new
    - chemical records
    - properties
    - data source records
    - data records
  - Retrieving data from the database

Chemical edit form

- This form allows you to enter and edit basic ID information about a chemical, including which data sources the chemical appears in

Property form

- In the property form it is possible to create and edit properties, viz. assigning which attributes are related to a particular property

Data source form

- Here it is possible to enter and edit data sources (databases, handbooks etc.)

New data form

- This is the form for entering and editing data for a certain chemical and property. It is possible to enter or edit data concerning the following details:
  - Chemical
  - Property
  - Experimental type
  - User
  - Database
  - Literature type
  - Year
  - Author
  - Attributes
  - Values

Data retrieval

- Using the report generator tool it is possible to select various kinds of reports with output to either MS Excel or in TAB-separated or an xml-format
- Example of reports:

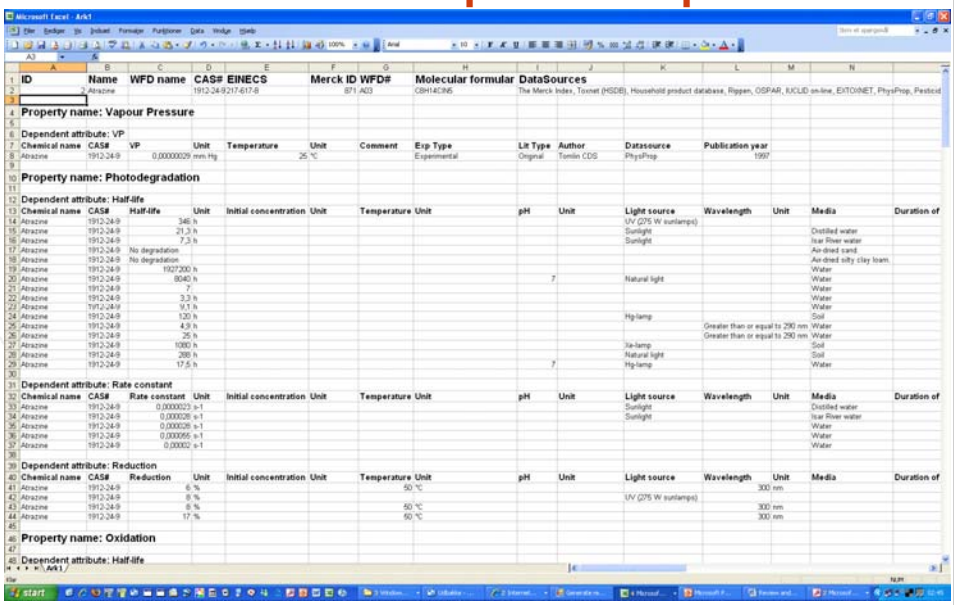
Chemical report

Property report

- Or just try the ReportGenerator which is included in this deliverable!

ReportGenerator procedure

Chemical report example



ID	Name	WFD name	CAS#	EINECS	Merck ID	WFD#	Molecular formular	DataSources
2	Atrazine		1912-24-9	217-617-8	871	A03	C8H14ClN5	The Merck Index, Toxnet (HSDB), Household product database, Ripper, OSPAR, IUCLID on-line, EXTOXNET, PhysProp, Pesticid

Property name: Vapour Pressure

Dependent attribute: VP

Chemical name	CAS#	VP	Unit	Temperature	Unit	Comment	Exp Type	Lit Type	Author	Datasource	Publication year
Atrazine	1912-24-9	0,00000029	mm Hg	25	°C		Experimental	Original	Tomlin CDS	PhysProp	1997

Property name: Photodegradation

Dependent attribute: Half-life

Chemical name	CAS#	Half-life	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	346	h							UV (275 W sunlamps)				
Atrazine	1912-24-9	21,3	h							Sunlight			Distilled water	
Atrazine	1912-24-9	7,3	h							Sunlight			Isar River water	
Atrazine	1912-24-9	No degradation											Air-dried sand	
Atrazine	1912-24-9	No degradation											Air-dried silty clay loam	
Atrazine	1912-24-9	1927200	h										Water	
Atrazine	1912-24-9	8040	h					7		Natural light			Water	
Atrazine	1912-24-9	7											Water	
Atrazine	1912-24-9	3,3	h										Water	
Atrazine	1912-24-9	9,1	h										Water	
Atrazine	1912-24-9	120	h							Hg-lamp			Soil	
Atrazine	1912-24-9	4,9	h								Greater than or equal to 290 nm		Water	
Atrazine	1912-24-9	25	h								Greater than or equal to 290 nm		Water	
Atrazine	1912-24-9	1060	h							Xe-lamp			Soil	
Atrazine	1912-24-9	288	h							Natural light			Soil	
Atrazine	1912-24-9	17,5	h					7		Hg-lamp			Water	

Dependent attribute: Rate constant

Chemical name	CAS#	Rate constant	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	0,0000023	s-1							Sunlight			Distilled water	
Atrazine	1912-24-9	0,000028	s-1							Sunlight			Isar River water	
Atrazine	1912-24-9	0,000026	s-1										Water	
Atrazine	1912-24-9	0,000055	s-1										Water	
Atrazine	1912-24-9	0,00002	s-1										Water	

Dependent attribute: Reduction

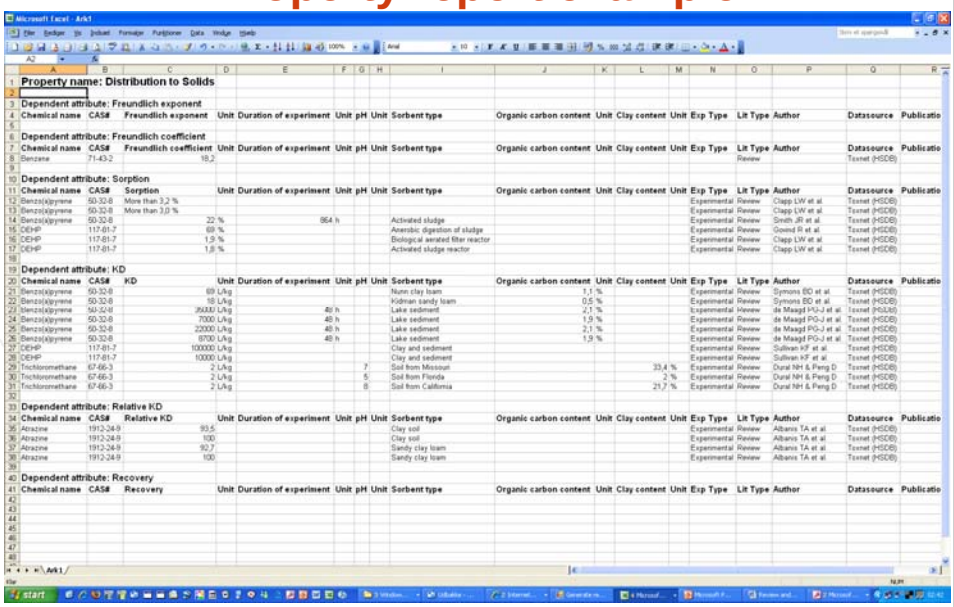
Chemical name	CAS#	Reduction	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	6	%			50	°C				300	nm		
Atrazine	1912-24-9	8	%							UV (275 W sunlamps)				
Atrazine	1912-24-9	8	%			50	°C				300	nm		
Atrazine	1912-24-9	17	%			50	°C				300	nm		

Property name: Oxidation

Dependent attribute: Half-life

Front page | Overview of PPT | Information collected | Substances in WFD | The database | Last slide viewed

Property report example



Property name: Distribution to Solids

Dependent attribute: Freundlich exponent

Chemical name	CAS#	Freundlich exponent	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio

Dependent attribute: Freundlich coefficient

Chemical name	CAS#	Freundlich coefficient	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzene	71-43-2	18,2												Review		Toxnet (HSDB)	

Dependent attribute: Sorption

Chemical name	CAS#	Sorption	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzo(a)pyrene	50-32-8	More than 3,2 %											Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	More than 3,0 %											Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	22 %		864 h				Activated sludge					Experimental	Review	Smith JR et al	Toxnet (HSDB)	
DEHP	117-81-7	69 %						Anerobic digestion of sludge					Experimental	Review	Govind R et al	Toxnet (HSDB)	
DEHP	117-81-7	1,9 %						Biological aerated filter reactor					Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
DEHP	117-81-7	1,8 %						Activated sludge reactor					Experimental	Review	Clapp LW et al	Toxnet (HSDB)	

Dependent attribute: KD

Chemical name	CAS#	KD	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzo(a)pyrene	50-32-8	69	L/kg					Nunn clay loam			1,1	%	Experimental	Review	Symons BD et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	18	L/kg					Kidman sandy loam			0,5	%	Experimental	Review	Symons BD et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	26400	L/kg			4	h	Lake sediment			2,1	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	7000	L/kg			48	h	Lake sediment			1,9	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	22000	L/kg			48	h	Lake sediment			2,1	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	8700	L/kg			48	h	Lake sediment			1,9	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
DEHP	117-81-7	100000	L/kg					Clay and sediment					Experimental	Review	Sullivan KF et al	Toxnet (HSDB)	
DEHP	117-81-7	10000	L/kg					Clay and sediment					Experimental	Review	Sullivan KF et al	Toxnet (HSDB)	
Trichloromethane	67-66-3	2	L/kg			7		Soil from Missouri			33,4	%	Experimental	Review	Dural NH & Peng D	Toxnet (HSDB)	
Trichloromethane	67-66-3	2	L/kg			5		Soil from Florida			2	%	Experimental	Review	Dural NH & Peng D	Toxnet (HSDB)	
Trichloromethane	67-66-3	2	L/kg			8		Soil from California			21,7	%	Experimental	Review	Dural NH & Peng D	Toxnet (HSDB)	

Dependent attribute: Relative KD

Chemical name	CAS#	Relative KD	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Atrazine	1912-24-9	93,5						Clay soil					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	100						Clay soil					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	92,7						Sandy clay loam					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	100						Sandy clay loam					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	

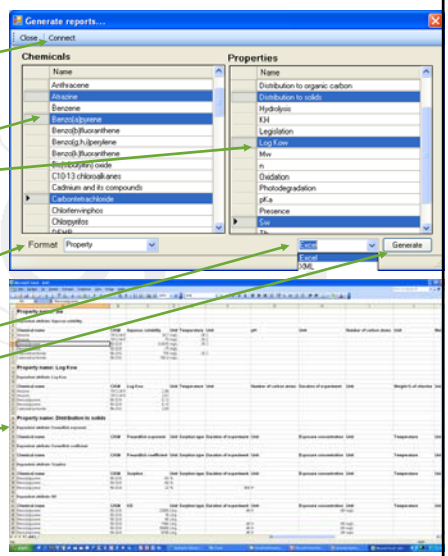
Dependent attribute: Recovery

Chemical name	CAS#	Recovery	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio

Front page | Overview of PPT | Information collected | Substances in WFD | The database | Last slide viewed

ReportGenerator procedure

- Click ”Connect” in the menue bar to select MS Access database (mdb)
- Select Chemical(s) and Property/ies for report in the 2 main panes
- Select report format
- Select output format
- Click ”Generate”
  - Report is generated



Software

- In order to retrieve data from the database the following software are required
  - MS Access; must be installed on the hard drive
  - MS.Net FrameWork 2.0; can be downloaded from: http://www.microsoft.com/downloads/details.aspx?FamilyID=0856EACB-4362-4B0D-8EDD-AAB15C5E04F5&displaylang=en
  - ReportGenerator; an add-on program enabling retrieval of data from the database (included in this deliverable) and which must be installed on the hard drive
  - MS Excel; the spreadsheet where the generated report can be viewed and handled

References

- **WFD: Decision No 2455/2001/EC of the European Parliament and of the Council of 20 November 2001 establishing the list of priority substances in the field of water policy and amending Directive 2000/60/EC:** http://europa.eu.int/eur-lex/pri/en/oj/dat/2001/l_331/l_33120011215en00010005.pdf
- **EQS: Proposal for a Directive of the European Parliament and of the Council on environmental quality standards in the field of water policy and amending Directive 2000/60/EC:** http://ec.europa.eu/environment/water/water-dangersub/pdf/-com_2006_397_en.pdf
- **ENVICAT Consulting, Avenue Montesquieu 36, B-1300 Wavre, Belgium**
- **US National Library of Medicine (2006). Hazardous Substance Data Bank (HSDB).** http://www.toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB

ScorePP is a Specific Targeted Research Project (STREP) funded by the European Commission under the Sixth Framework

Source Control Options for Reducing Emissions of Priority Pollutants (ScorePP)

D3.1 Short introduction to using the ”Database Presenting basic Information about EU WFD Priority Substances

Contents of this presentation

General Information

Specific Information

Guidelines on how to operate the database

Contents of This Presentation

- General and specific remarks to the output of the database
  - The reader must pay attention to that not all data reported have equal amounts of information related to the experimental conditions
  - Regarding data on vapour pressure, the reported values are not always in the same unit
- Guidelines on how to operate the database
  - Introduction to which data can be put in the database and how data are entered in the database

General Information

- In general, the aim has been to compile property information with as many details about the experimental conditions as possible. Therefore the different properties will, in some cases, be accompanied with information about e.g. experimental temperature, pH, pressure, sorbent type etc. Sometimes there will be a lot of accompanying information and sometimes there will be none. In the cases that no accompanying information is given, we think this is actually also valuable information, as one therefore will know that no further details about the experiment are known.
- If one is retrieving data on one property for one or more substances, one actually has the opportunity to select among the accompanying information.

Specific Information

- Data on vapour pressure might be given in different units, e.g. mmHg and mPa. The SI unit for pressure is Pa, where a standard atmosphere, 1 atm or 760 mmHg, equals 101.325 Pa. For that purpose Table 1 below gives the possibility to convert mmHg, mPa and hPa into the SI unit:

Table 1 – Equations used to convert pressure from various units into the SI unit.

Pressure in	equation used for conversion
mmHg	P Pa = P mmHg x 133,322 Pa/mmHg
mPa	P Pa = P mPa x 10^{-3} Pa/mPa
hPa	P Pa = P hPa x 100 Pa/hPa

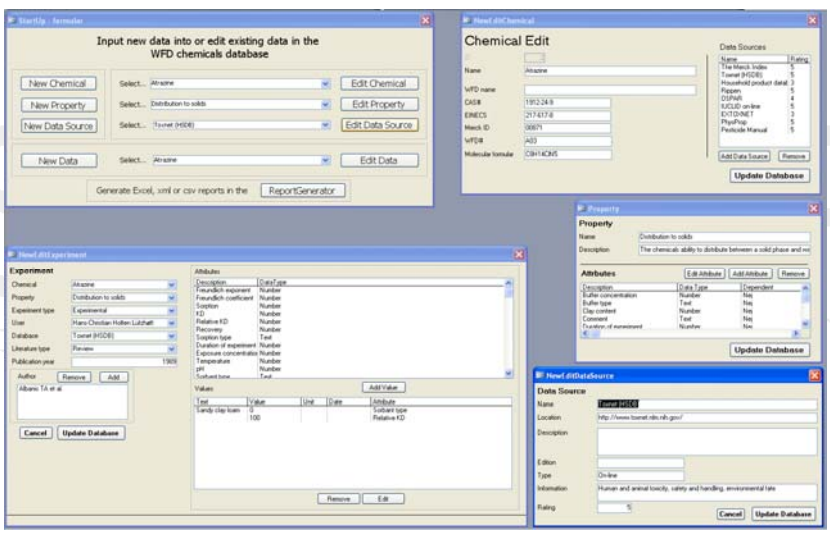
Guidelines on how to operate the database

Data entry

Data retrieval

Software

Data entry



Click on a form to get more information!

Main entry form

- This form presents the various possibilities in the database
  - Selecting records for review or editing on
    - existing chemicals
    - properties
    - data sources
    - data
  - Creating new
    - chemical records
    - properties
    - data source records
    - data records
  - Retrieving data from the database

Chemical edit form

- This form allows you to enter and edit basic ID information about a chemical, including which data sources the chemical appears in

Property form

- In the property form it is possible to create and edit properties, viz. assigning which attributes are related to a particular property

Data source form

- Here it is possible to enter and edit data sources (databases, handbooks etc.)

New data form

- This is the form for entering and editing data for a certain chemical and property. It is possible to enter or edit data concerning the following details:
  - Chemical
  - Property
  - Experimental type
  - User
  - Database
  - Literature type
  - Year
  - Author
  - Attributes
  - Values

Data retrieval

- Using the report generator tool it is possible to select various kinds of reports with output to either MS Excel or in TAB-separated or an xml-format
- Examples of reports:

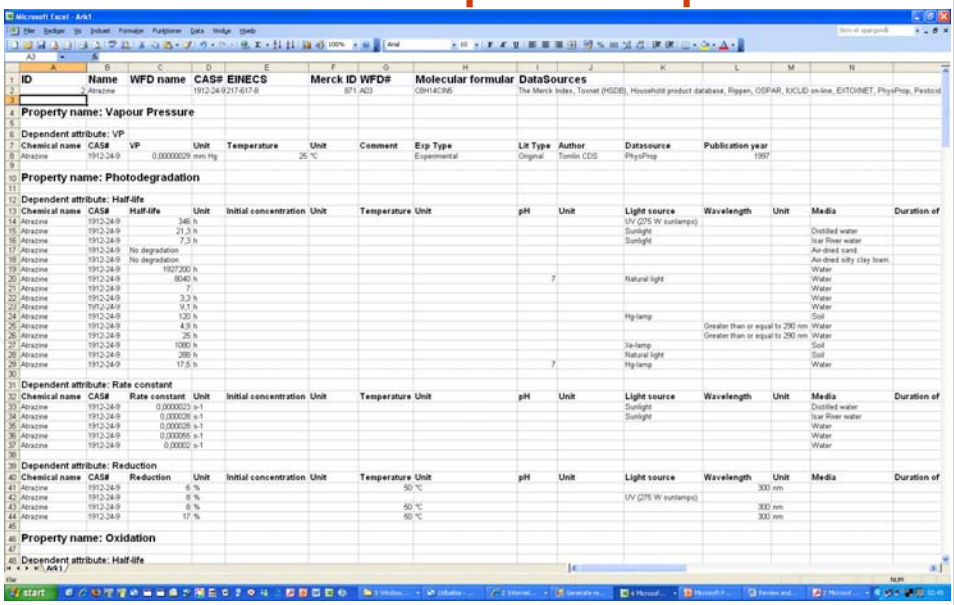
Chemical report

Property report

- Or just try the ReportGenerator which is included in this deliverable!

ReportGenerator procedure

Chemical report example



ID	Name	WFD name	CAS#	EINECS	Merck ID	WFD#	Molecular formular	DataSources
2	Atrazine		1912-24-9	217-617-8	871	A03	C8H14ClN5	The Merck Index, Toxnet (HSDB), Household product database, Ripper, OSPAR, IUCLID on-line, EXTOXNET, PhysProp, Pesticid

Property name: Vapour Pressure

Dependent attribute: VP

Chemical name	CAS#	VP	Unit	Temperature	Unit	Comment	Exp Type	Lit Type	Author	Datasource	Publication year
Atrazine	1912-24-9	0,00000029	mm Hg	25	°C		Experimental	Original	Tomlin CDS	PhysProp	1997

Property name: Photodegradation

Dependent attribute: Half-life

Chemical name	CAS#	Half-life	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	346	h							UV (275 W sunlamps)				
Atrazine	1912-24-9	21,3	h							Sunlight			Distilled water	
Atrazine	1912-24-9	7,3	h							Sunlight			Isar River water	
Atrazine	1912-24-9	No degradation											Air-dried sand	
Atrazine	1912-24-9	No degradation											Air-dried silty clay loam	
Atrazine	1912-24-9	1927200	h										Water	
Atrazine	1912-24-9	8040	h					7		Natural light			Water	
Atrazine	1912-24-9	7											Water	
Atrazine	1912-24-9	3,3	h										Water	
Atrazine	1912-24-9	9,1	h										Water	
Atrazine	1912-24-9	120	h							Hg-lamp			Soil	
Atrazine	1912-24-9	4,9	h								Greater than or equal to 290 nm		Water	
Atrazine	1912-24-9	25	h								Greater than or equal to 290 nm		Water	
Atrazine	1912-24-9	1060	h							Xe-lamp			Soil	
Atrazine	1912-24-9	288	h							Natural light			Soil	
Atrazine	1912-24-9	17,5	h					7		Hg-lamp			Water	

Dependent attribute: Rate constant

Chemical name	CAS#	Rate constant	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	0,0000023	s-1							Sunlight			Distilled water	
Atrazine	1912-24-9	0,000028	s-1							Sunlight			Isar River water	
Atrazine	1912-24-9	0,000026	s-1										Water	
Atrazine	1912-24-9	0,000055	s-1										Water	
Atrazine	1912-24-9	0,00002	s-1										Water	

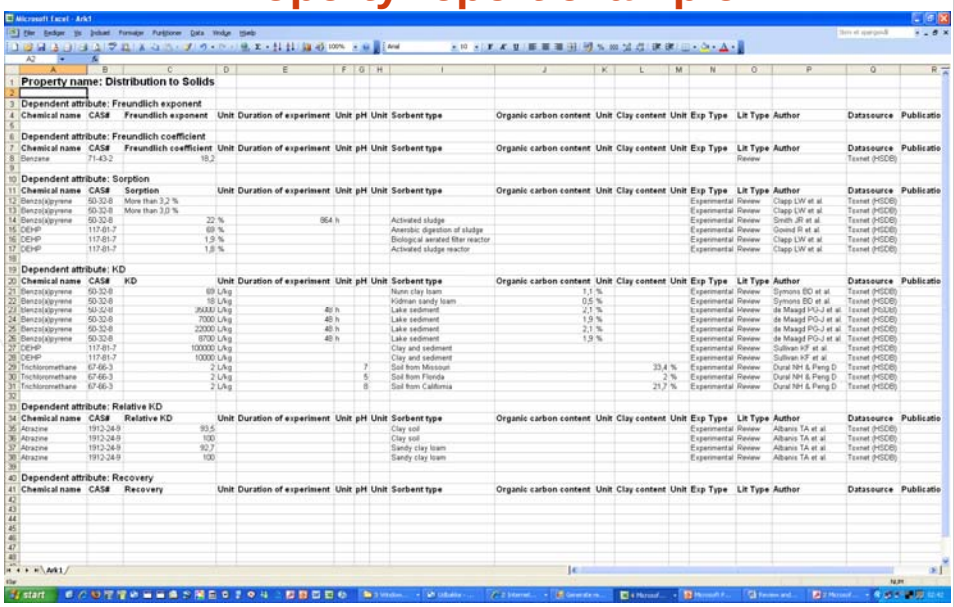
Dependent attribute: Reduction

Chemical name	CAS#	Reduction	Unit	Initial concentration	Unit	Temperature	Unit	pH	Unit	Light source	Wavelength	Unit	Media	Duration of
Atrazine	1912-24-9	6	%			50	°C				300	nm		
Atrazine	1912-24-9	8	%							UV (275 W sunlamps)				
Atrazine	1912-24-9	8	%			50	°C				300	nm		
Atrazine	1912-24-9	17	%			50	°C				300	nm		

Property name: Oxidation

Dependent attribute: Half-life

Property report example



Property name: Distribution to Solids

Dependent attribute: Freundlich exponent

Chemical name	CAS#	Freundlich exponent	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio

Dependent attribute: Freundlich coefficient

Chemical name	CAS#	Freundlich coefficient	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzene	71-43-2	18,2												Review		Toxnet (HSDB)	

Dependent attribute: Sorption

Chemical name	CAS#	Sorption	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzo(a)pyrene	50-32-8	More than 3,2 %											Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	More than 3,0 %											Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	22 %		864 h				Activated sludge					Experimental	Review	Smith JR et al	Toxnet (HSDB)	
DEHP	117-81-7	69 %						Anerobic digestion of sludge					Experimental	Review	Govind R et al	Toxnet (HSDB)	
DEHP	117-81-7	1,9 %						Biological aerated filter reactor					Experimental	Review	Clapp LW et al	Toxnet (HSDB)	
DEHP	117-81-7	1,8 %						Activated sludge reactor					Experimental	Review	Clapp LW et al	Toxnet (HSDB)	

Dependent attribute: KD

Chemical name	CAS#	KD	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Benzo(a)pyrene	50-32-8	69	L/kg					Nunn clay loam			1,1	%	Experimental	Review	Symons BD et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	18	L/kg					Kidman sandy loam			0,5	%	Experimental	Review	Symons BD et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	26400	L/kg			4	hr	Lake sediment			2,1	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	7000	L/kg			48	h	Lake sediment			1,9	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
Benzo(a)pyrene	50-32-8	22000	L/kg			48	h	Lake sediment			2,1	%	Experimental	Review	de Maagd PG-J et al	Toxnet (HSDB)	
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DEHP	117-81-7	100000	L/kg					Clay and sediment					Experimental	Review	Sullivan KF et al	Toxnet (HSDB)	
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Trichloromethane	67-66-3	2	L/kg			7		Soil from Missouri			33,4	%	Experimental	Review	Dural NH & Peng D	Toxnet (HSDB)	
Trichloromethane	67-66-3	2	L/kg			5		Soil from Florida			2	%	Experimental	Review	Dural NH & Peng D	Toxnet (HSDB)	
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Dependent attribute: Relative KD

Chemical name	CAS#	Relative KD	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio
Atrazine	1912-24-9	93,5						Clay soil					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	100						Clay soil					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	92,7						Sandy clay loam					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	
Atrazine	1912-24-9	100						Sandy clay loam					Experimental	Review	Albanis TA et al	Toxnet (HSDB)	

Dependent attribute: Recovery

Chemical name	CAS#	Recovery	Unit	Duration of experiment	Unit	pH	Unit	Sorbent type	Organic carbon content	Unit	Clay content	Unit	Exp Type	Lit Type	Author	Datasource	Publicatio

ReportGenerator procedure

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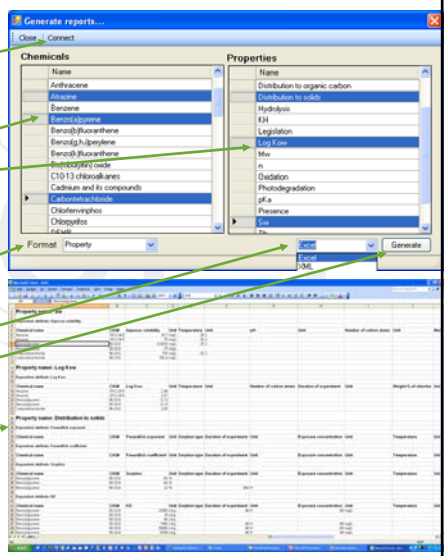

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  - ReportGenerator; an add-on program enabling retrieval of data from the database (included in this deliverable) and which must be installed on the hard drive
  - MS Excel; the spreadsheet where the generated report can be viewed and handled